Pentanedioic acid, hexafluoro-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.02

Global applicability domain: Inside

Local applicability domain index: 4.66e-01

Confidence level: 7.72e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl perfluoropropionate
Measured: 2.12
Predicted: 2.04

Image not found
Benzene, (trimethoxymethyl)-
Measured: 2.27
Predicted: 2.03

Image not found
1-Butanol, 2,2,3,3,4,4,4-heptafluoro-
Measured: 1.94
Predicted: 1.93

Image not found
2-[2-(Hexyloxy)ethoxy]ethanol
Measured: 1.70
Predicted: 1.54

Image not found
2-(diethylamino)-1-phenylethanol
Measured: 2.02
Predicted: 1.83